

THE INFINITE ARNOLDI EXPONENTIAL INTEGRATOR FOR LINEAR INHOMOGENEOUS ODES

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Abstract. Exponential integrators that use Krylov approximations of matrix functions have turned out to be efficient for the time-integration of certain ordinary differential equations (ODEs). This holds in particular for linear homogeneous ODEs, where the exponential integrator is equivalent to approximating the product of the matrix exponential and a vector. In this paper, we consider linear inhomogeneous ODEs, $y'(t) = Ay(t) + g(t)$, where the function $g(t)$ is assumed to satisfy certain regularity conditions. We derive an algorithm for this problem which is equivalent to approximating the product of the matrix exponential and a vector using Arnoldi's method. The construction is based on expressing the function $g(t)$ as a linear combination of given basis functions $[\phi_i]_{i=0}^\infty$ with particular properties. The properties are such that the inhomogeneous ODE can be restated as an infinite-dimensional linear homogeneous ODE. Moreover, the linear homogeneous infinite-dimensional ODE has properties that directly allow us to extend a Krylov method for finite-dimensional linear ODEs. Although the construction is based on an infinite-dimensional operator, the algorithm can be carried out with operations involving matrices and vectors of finite size. This type of construction resembles in many ways the infinite Arnoldi method for nonlinear eigenvalue problems [15]. We prove convergence of the algorithm under certain natural conditions, and illustrate properties of the algorithm with examples stemming from the discretization of partial differential equations.

Key words. Arnoldi's method, exponential integrators, matrix functions, ordinary differential equations, Bessel functions

AMS subject classifications. 65F10, 65F60, 65L05, 65L20

DOI.

1. Introduction. Consider a matrix $A \in \mathbb{C}^{n \times n}$ and a function $g : \mathbb{C} \rightarrow \mathbb{C}^n$ with elements which are entire functions. We consider the problem of numerically computing the time-evolution of the linear ordinary differential equation with an inhomogeneous term

$$u'(t) = Au(t) + g(t), \quad u(0) = u_0. \quad (1.1)$$

Our focus will be on equations that arise from spatial semidiscretization of partial differential equations of evolutionary type, and A will typically be a large sparse matrix, and g will neither be close to linear nor correspond to an extremely stiff nonlinearity, in a sense which is further explained in the examples in Section 5.

The general problem of computing the time-evolution of ODEs can be approached with various numerical methods. The method we will present in this paper belongs to the class of methods called *exponential integrators*. Exponential integrators have recently received considerable interest; see the review paper [14]. An attractive feature of these methods stems from the combination of approximation of matrix functions and the use of Krylov methods [13]. This is mostly due to the superlinear convergence of the Krylov approximation of entire matrix functions [12].

In this paper we will present a new exponential integrator for (1.1). The integrator is constructed using a particular type of expansion of the function g in (1.1). We will

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consider expansions of the type

$$g(s) = \sum_{\ell=0}^{\infty} w_{\ell} \phi_{\ell}(s), \quad (1.2)$$

where $w_{\ell} \in \mathbb{C}^n$, $\ell \in \mathbb{N}$, and the basis functions ϕ_0, ϕ_1, \dots are assumed to satisfy

$$\frac{d}{dt} \begin{bmatrix} \phi_0(t) \\ \phi_1(t) \\ \vdots \end{bmatrix} = H_{\infty} \begin{bmatrix} \phi_0(t) \\ \phi_1(t) \\ \vdots \end{bmatrix}, \quad \begin{bmatrix} \phi_0(0) \\ \phi_1(0) \\ \vdots \end{bmatrix} = e_1 \quad (1.3a)$$

where $H_{\infty} \in \mathbb{R}^{\infty \times \infty}$ is an infinite-dimensional Hessenberg matrix, satisfying for a fixed constant $C \geq 0$,

$$\|H_N\| < C \text{ for all } N = 0, \dots, \infty. \quad (1.3b)$$

The matrix $H_N \in \mathbb{R}^{N \times N}$ is the leading submatrix of H_{∞} .

The scaled monomials is the easiest example of such a sequence of functions. If we define $\phi_{\ell}(t) := t^{\ell}/\ell!$, $i = 0, \dots$, then (1.3) is satisfied with H_{∞} given by a transposed Jordan matrix

$$H_{\infty} = \begin{bmatrix} 0 & & & \\ 1 & 0 & & \\ & 1 & 0 & \\ & & \ddots & \ddots \end{bmatrix}. \quad (1.4)$$

In this case, the expansion (1.2) corresponds to a Taylor expansion and the coefficients are given by $w_{\ell} = g^{(\ell)}(0)$, $\ell = 0, \dots$. We will also see that these properties are satisfied for other functions, e.g., the Bessel function and the modified Bessel function of the first kind (as we will further explain in Section 2.2). The algorithm will be derived and analyzed for these choices of $[\phi_i]_{i=0}^{\infty}$. The choice of basis functions can be tailored for the problem, and the best choice is problem dependent. This will be illustrated in the numerical examples in Section 5.

The general idea of our approach can be seen as follows. If ϕ_0, ϕ_1, \dots are the scaled monomials, then we can truncate (1.2) at $\ell = N$, yielding $\tilde{y}'(t) = A\tilde{y}(t) + \sum_{\ell=0}^{N-1} w_{\ell} \phi_{\ell}(t)$ and it straightforward to verify that the inhomogeneous ODE (1.1) can be expressed as a larger linear homogeneous ODE,

$$\frac{d}{dt} \begin{bmatrix} \tilde{y}(t) \\ \phi_0(t) \\ \vdots \\ \phi_{N-1}(t) \end{bmatrix} = A_N \begin{bmatrix} \tilde{y}(t) \\ \phi_0(t) \\ \vdots \\ \phi_{N-1}(t) \end{bmatrix}, \quad \begin{bmatrix} y(0) \\ \phi_0(0) \\ \vdots \\ \phi_{N-1}(0) \end{bmatrix} = \begin{bmatrix} y_0 \\ e_1 \end{bmatrix} \quad (1.5)$$

where we have defined

$$A_N := \begin{bmatrix} A & W_N \\ 0 & H_N \end{bmatrix} \quad (1.6)$$

and $H_N \in \mathbb{R}^{N \times N}$ is the leading $N \times N$ block of H_{∞} and $W_N := [w_0 \ \dots \ w_{N-1}] \in \mathbb{C}^{n \times N}$. This relation has been used in [2, Theorem 2.1] and also in [16]. If we combine this type of construction with an iterative method (in a particular way), we will here

be able to construct an algorithm for (1.1) for any sequence of functions ϕ_0, ϕ_1, \dots satisfying (1.3).

The construction (1.5) and the matrix (1.6) resemble in some ways the technique called companion linearization used for polynomial eigenvalue problems; see e.g. [17, 21]. The algorithm known as the infinite Arnoldi method [15] is an algorithm for nonlinear eigenvalue problems (not necessarily polynomial). One variant of the infinite Arnoldi method can be interpreted as the Arnoldi method [20] applied to the companion linearization of a truncated Taylor expansion. Due to a particular structure of the companion matrix, the infinite Arnoldi method is also equivalent to the application of the Arnoldi method on an infinite-dimensional companion matrix. This equivalence is consistent with the observation that many attractive features of the Arnoldi method appear to be present also in the infinite Arnoldi method.

We will in this paper illustrate that the underlying techniques used to derive the infinite Arnoldi method can also be applied to (1.1). Similar to the infinite Arnoldi method, the presented algorithm can be interpreted as an exponential integrator applied to a truncated problem, as well as the integrator applied to an infinite-dimensional problem. An important feature of this construction is that the algorithm does not require a choice of a truncation parameter in the expansion (1.2), making it in a sense applicable to arbitrary nonlinearities.

The paper is structured as follows. The infinite-dimensional properties of the algorithm are derived in Section 2.1. Although the construction in Section 2.1 is general for essentially arbitrary basis, the convergence proofs are basis dependent. We show that the algorithm converges for several bases (scaled monomials, Bessel functions and modified Bessel functions) under certain conditions, i.e., the truncation of (1.2) converges and the derivatives $g^{(\ell)}(0)$ of the nonlinearity are bounded with respect to the linear operator A in a certain way. This convergence theory is presented in Section 4. We illustrate the properties of the algorithm and its variants in Section 5 including comparisons with other algorithms.

We will mostly use standard notation. $(H_N)_{i,j}$ denotes the element at the i th row and j th column of H_N . Analogously, the colon notation will be used to denote entire rows and columns, e.g., $V_{k,:}$ corresponds to the vector in the k th row of the matrix V . We will also extensively use infinite-dimensional matrices. More precisely, we will work with sequences of matrices $W_N \in \mathbb{R}^{n \times N}$, $N = 0, \dots$, which are nested, i.e., $W_{N-1} \in \mathbb{R}^{n \times (N-1)}$ are the first $N - 1$ columns of W_N , and W_∞ will be the corresponding infinite-dimensional matrix. We will also consider sequences of square matrices $H_N \in \mathbb{R}^{N \times N}$, where H_{N-1} is the leading submatrix of H_N . The infinite-dimensional operator associated with the limit will be denoted $H_\infty \in \mathbb{R}^{\infty \times \infty}$. We will use e_i to denote the i th unit vector of consistent size. Throughout the paper, $\|\cdot\|$ denotes the Euclidean vector norm or the spectral matrix norm, unless otherwise stated.

2. Preliminaries.

2.1. Infinite-dimensional reformulation. At first we will show that the inhomogeneous ODE (1.1) is equivalent to an infinite-dimensional homogeneous ODE. The reformulation is illustrated in the following lemma and can be interpreted as an analogous transformation illustrated for monomials and truncated Taylor expansion in (1.5) and (1.6), but without truncation and for arbitrary basis functions satisfying (1.3).

Lemma 1 (Infinite-dimensional reformulation) Consider the initial value problem (1.1), and a sequence of basis functions $[\phi_i]_{i=0}^{\infty}$ which satisfy (1.3). Moreover, suppose that the function g in (1.1) can be expanded as (1.2), and let $W_{\infty} = [w_0, w_1, w_2, \dots] \in \mathbb{C}^{n \times \infty}$ denote the expansion coefficients.

(a) Suppose $u(t)$ is a solution to (1.1). Then

$$\frac{d}{dt} \begin{bmatrix} u \\ \phi_0 \\ \vdots \end{bmatrix} = \begin{bmatrix} A & W_{\infty} \\ 0 & H_{\infty} \end{bmatrix} \begin{bmatrix} u \\ \phi_0 \\ \vdots \end{bmatrix}, \quad \begin{bmatrix} u(0) \\ \phi_0(0) \\ \vdots \end{bmatrix} = \begin{bmatrix} u_0 \\ e_1 \\ \vdots \end{bmatrix}. \quad (2.1)$$

(b) Suppose $v(t)$ satisfies

$$v'(t) = \begin{bmatrix} A & W_{\infty} \\ 0 & H_{\infty} \end{bmatrix} v(t), \quad v(0) = \begin{bmatrix} u_0 \\ e_1 \\ \vdots \end{bmatrix}. \quad (2.2)$$

Then the function $u(t) := [I_n \ 0] v(t)$ is the unique solution to (1.1).

Proof. The equation (2.1) is easily verified by considering the individual blocks. The first n rows of (2.1) satisfy $u'(t) = Au(t) + \sum_{\ell=0}^{\infty} W_{\ell} \phi_{\ell}(t) = Au(t) + g(t)$. Rows $n+1, n+2, \dots$ are precisely the conditions in (1.3a). In order to show (2.2), first note that the rows $n+1, n+2, \dots$ in (2.2) reduce to the equation

$$\frac{d}{dt} \begin{bmatrix} v_{n+1}(t) \\ \vdots \end{bmatrix} = H_{\infty} \begin{bmatrix} v_{n+1}(t) \\ \vdots \end{bmatrix}, \quad \begin{bmatrix} v_{n+1}(0) \\ \vdots \end{bmatrix} = e_1.$$

Since the operator H_{∞} has a finite norm by assumption (1.3b), it follows from the Picard-Lindelöf theorem that there exists a unique solution. This solution is the sequence of basis functions ϕ_0, ϕ_1, \dots , since they satisfy this ODE by assumption, i.e., $v_{n+1+i} = \phi_i$ for all $i \in \mathbb{N}$. The conclusion follows by substituting $v(t)$ into the first n rows in (2.2). \square

2.2. Characterization of basis functions ϕ_{ℓ} . As mentioned in the introduction (in particular in formula (1.4)), it is straightforward to verify that the scaled monomials satisfy the condition (1.3) required for the basis functions. Although the algorithm described in the following section applies for any basis functions satisfying (1.3), we concentrate the discussion on specialized results for two additional types of functions. We will now show that the Bessel functions and the modified Bessel functions of the first kind satisfy (1.3).

The Bessel functions of the first kind are defined by (see e.g. [1]), $J_{\ell}(t) := \frac{1}{\pi} \int_0^{\pi} \cos(\ell\tau - t \sin(\tau)) d\tau$, for $\ell \in \mathbb{N}$, and they satisfy

$$J'_{\ell}(t) = \frac{1}{2} (J_{\ell-1}(t) - J_{\ell+1}(t)). \quad (2.3a)$$

$$J_{-\ell}(t) = (-1)^{\ell} J_{\ell}(t), \quad \ell > 0 \quad (2.3b)$$

$$J_{\ell}(0) = \begin{cases} 1 & \text{if } \ell = 0 \\ 0 & \text{otherwise} \end{cases}. \quad (2.3c)$$

Let $\bar{J}_N(t) = [J_0(t) \ J_1(t) \ \dots \ J_{N-1}(t)]^T \in \mathbb{R}^N$, i.e., a vector of Bessel functions

with non-negative index. Moreover, let

$$H_N = \begin{bmatrix} 0 & -1 & & & \\ \frac{1}{2} & 0 & -\frac{1}{2} & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & 0 & -\frac{1}{2} \\ & & & \frac{1}{2} & 0 \end{bmatrix} \in \mathbb{C}^{N \times N}. \quad (2.4)$$

From the relations (2.3), we easily verify that the Bessel functions of the first kind are solutions to the infinite-dimensional ODE of the form (1.3), with H_N given by (2.4). More precisely,

$$\bar{J}'_\infty(t) = H_\infty \bar{J}_\infty(t), \quad \bar{J}_\infty(0) = e_1.$$

With similar reasoning we can establish an ODE (1.3) also for the modified Bessel functions of the first kind, which are defined by

$$I_\ell(t) := (-i)^n J_n(it). \quad (2.5)$$

and satisfy $I'_\ell(t) = \frac{1}{2}(I_{\ell-1}(t) + I_{\ell+1}(t))$, $\ell \in \mathbb{N}$. These properties lead to the infinite-dimensional ODE

$$\bar{I}'_\infty(t) = H_\infty \bar{I}_\infty(t), \quad I(0) = e_1,$$

where $\bar{I}_N(t) = [I_0(t) \quad I_1(t) \quad \dots \quad I_{N-1}(t)]^T$ and

$$H_N = \begin{bmatrix} 0 & 1 & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & 0 & \frac{1}{2} \\ & & & \frac{1}{2} & 0 \end{bmatrix} \in \mathbb{C}^{N \times N}. \quad (2.6)$$

Therefore, we can show that the Bessel functions and the modified Bessel functions of the first kind satisfy (1.3), with an explicitly given constant C .

Lemma 2 (Basis functions) *The conditions for the basis functions in (1.3) are satisfied with $C = 2$ for,*

- (a) *scaled monomials, i.e., $\phi_i(t) = t!/i!$, with H_∞ defined by (1.4);*
- (b) *Bessel functions, i.e., $\phi_i(t) = J_i(t)$, with H_∞ defined by (2.4); and*
- (c) *modified Bessel functions, i.e., $\phi_i(t) = I_i(t)$, with H_∞ defined by (2.6).*

Proof. Statement (a) follows from the definition. The conditions (1.3a) have been shown already for (b) and (c), since they follow directly from (2.3) and (2.5). It remains to show that the uniform bound (1.3b) is satisfied for (b) and (c). Note that in both cases (b) and (c) we can express H_N as $H_N = T_N + E_N$, where $E_N = \pm \frac{1}{2}e_1 e_2^T$ and T_N is a (finite) band Toeplitz matrix, for any $N = 2, \dots, \infty$. We now invoke a general result for (finite) band Toeplitz matrices [5, Theorem 1.1] which implies that $\|T_N\| \leq \|T_\infty\| = 1$. Hence, $\|H_N\| \leq \|T_N\| + \|E_N\| = 3/2$, and (1.3b) holds with $C = 2$. \square

2.3. Characterization of expansion coefficients w_ℓ . In principle, the algorithm will be applicable to any problem for which there is a convergent expansion of the form (1.2) with some coefficients $w_\ell \in \mathbb{C}^n$, $\ell \in \mathbb{N}$. In practice these coefficients may not be explicitly available. We will now characterize a relationship between the coefficients and the derivatives of g . This will be necessary in the theoretical convergence analysis in Section 4 and also useful in numerical evaluation of the coefficients (Section 5).

Assume that an expansion of the form (1.2) exists and let

$$W_N = [w_0 \quad w_1 \quad \dots \quad w_{N-1}] .$$

By considering the ℓ th derivative of $g(t)$ and using the properties of basis functions (1.3) we have that

$$g^{(\ell)}(0) = W_\infty H_\infty^\ell e_1 = W_N H_N^\ell e_1 \quad \text{for all } \ell < N.$$

In the last equality we used the fact that H_∞ is a Hessenberg matrix, and that all elements of $H_\infty^\ell e_1$ except the first $\ell + 1$ elements will be zero. The non-zero elements will also be equal to $H_N^\ell e_1$. We now define the upper-triangular matrix

$$K_N(H_N, e_1) = [e_1 \quad H_N e_1 \quad \dots \quad H_N^{N-1} e_1] , \quad (2.7)$$

and the matrix G_N as

$$G_N = [g(0) \quad g'(0) \quad \dots \quad g^{(N-1)}(0)] . \quad (2.8)$$

From the definition it follows that

$$W_N = G_N K_N(H_N, e_1)^{-1} \quad \text{for all } N \geq 1, \quad (2.9)$$

under the condition that $K_N(H_N, e_1)$ is invertible. In a generic situation, the relation (2.9) can be directly used to compute the coefficients w_ℓ , $\ell \in \mathbb{N}$, given the derivatives of $g(t)$. For the Bessel functions and the modified Bessel functions of the first kind, we can characterize the coefficients with a more explicit (and more numerically robust) formula involving the monomial coefficients of the Chebyshev polynomials of the first kind.

Lemma 3 Let $T_{k,\ell}$ be the monomial coefficients of the k th Chebyshev polynomial, i.e., $T_k(x) = \sum_{\ell=0}^k T_{k,\ell} x^\ell$.

- (a) For scaled monomials, i.e., $\phi_k(t) = t!/k!$, the expansion coefficients are given by $w_k = g^{(k)}(0)$, for $k \in \mathbb{N}$.
- (v) For the Bessel functions of the first kind, i.e., $\phi_\ell(t) = J_\ell(t)$, the expansion coefficients w_ℓ are given by,

$$w_0 = g(0), \quad w_k = 2 \sum_{\ell=0}^k (-1)^\ell T_{k,\ell} g^{(\ell)}(0), \quad k = 1, \dots .$$

- (c) For the modified Bessel functions of the first kind, i.e., $\phi_\ell(t) = I_\ell(t)$, the expansion coefficients w_ℓ are given by,

$$w_0 = g(0), \quad w_k = 2 \sum_{\ell=0}^k T_{k,\ell} g^{(\ell)}(0), \quad k = 1, \dots .$$

Proof. Case (a) follows from the definition. Consider case (c) with the modified Bessel functions, i.e., let H_N be given by (2.6). The proof is based on showing that

$$K_N(H_N, e_1)^{-1} = 2 \begin{bmatrix} \frac{1}{2}T_{0,0} & T_{1,0} & \cdots & T_{N-1,0} \\ 0 & T_{1,1} & & T_{N-1,1} \\ \vdots & & \ddots & \vdots \\ 0 & & \cdots & T_{N-1,N-1} \end{bmatrix}, \quad (2.10)$$

from which the conclusion follows directly from (2.9) and the fact that $T_{k,k} = 2^{k-1}$ for any $k > 0$.

We will first prove (2.10) for columns $k = 2, 3, \dots, N$. From (2.7) and (2.6) we directly identify that

$$K_{N+1}(H_{N+1}, e_1) = \begin{bmatrix} K_N(H_N, e_1) & H_N^N e_1 \\ 0 & 2^{-N} \end{bmatrix}.$$

Moreover, by explicitly formulating the Schur complement [8, Section 3.2.11] we have that

$$K_{N+1}(H_{N+1}, e_1)^{-1} = \begin{bmatrix} K_N(H_N, e_1)^{-1} & -2^N K_N(H_N, e_1)^{-1} H_N^N e_1 \\ 0 & 2^N \end{bmatrix}. \quad (2.11)$$

Now let $p_N(\lambda)$ be the characteristic polynomial of H_N , i.e., $p_N(\lambda) = \det(\lambda I - H_N)$.

By expanding the determinant of $\lambda I - H_N$ for the last row, we find that

$$p_N(\lambda) = \lambda p_{N-1}(\lambda) - \frac{1}{4} p_{N-2}(\lambda). \quad (2.12)$$

Now let $\tilde{p}_N(\lambda) := 2^{N-1} p_N(\lambda)$ which satisfies the recursion $\tilde{p}_N(\lambda) = 2\lambda \tilde{p}_{N-1}(\lambda) - \tilde{p}_{N-2}(\lambda)$. This is exactly the recursion of the Chebyshev polynomials. We have $\tilde{p}_1(\lambda) = \lambda = T_1(\lambda)$ and $\tilde{p}_2(\lambda) = (2\lambda^2 - 1) = T_2(\lambda)$. Hence, by induction starting with $N = 1$ and $N = 2$ it follows that $\tilde{p}_N(\lambda) = T_N(\lambda)$, for all $N \geq 1$. Note that $\tilde{p}_0 \neq T_0$. The Cayley-Hamilton theorem implies that $0 = p_N(H_N) = \tilde{p}_N(H_N) = T_N(H_N)$ and in particular $0 = 2\tilde{p}(H_N)e_1$, i.e.,

$$-2^N H_N^N e_1 = \sum_{i=0}^{N-1} 2T_{N,i} H_N^i e_1. \quad (2.13)$$

The first N rows of the last column of (2.11) can now be expressed as

$$-2^N K_N(H_N, e_1)^{-1} H_N^N e_1 = 2K_N(H_N, e_1)^{-1} \left(\sum_{i=0}^{N-1} T_{N,i} H_N^i e_1 \right) = 2 \begin{bmatrix} T_{N,0} \\ \vdots \\ T_{N,N-1} \end{bmatrix}$$

The structure in (2.10) for columns $k = 2, \dots, N$ follows by induction. The first column can be verified directly by noting that $K_1(H_1, e_1) = 1 = T_{0,0}$.

The proof for the case (b) goes analogously. From (2.6) we see that in this case the characteristic polynomial $p_N(\lambda)$ of H_N satisfies the recursion

$$p_N(\lambda) = \lambda p_{N-1}(\lambda) + \frac{1}{4} p_{N-2}(\lambda). \quad (2.14)$$

Defining $\tilde{p}_N(\lambda) = 2^{N-1} p_N(\lambda)$ and writing out the recursions we find (similarly to the case (c)) that $\tilde{p}_N(\lambda) = (-i)^N T_N(i\lambda)$. Comparing (2.12) and (2.14) we see that $\tilde{p}_N(\lambda)$ is of the form $\tilde{p}_N(\lambda) = \sum_{\ell=0}^N |T_{N,\ell}| \lambda^\ell$. The claim follows from this. \square

Remark 4 (Combining with formulas for the Chebyshev polynomials) The coefficients $T_{k,\ell}$ are given by the explicit expression (see [1, pp. 775])

$$T_k(x) = \sum_{\ell=0}^{\lfloor \frac{k}{2} \rfloor} (-1)^\ell \frac{k(k-\ell-1)!}{\ell!(k-2\ell)!} 2^{k-2\ell-1} x^{k-2\ell}. \quad (2.15)$$

Thus, when the basis functions ϕ_ℓ are the modified Bessel functions of the first kind, the coefficients of the expansion (1.2) are explicitly given by

$$\begin{aligned} w_k &= \sum_{\ell=0}^{\lfloor \frac{k}{2} \rfloor} (-1)^\ell \frac{k(k-\ell-1)!}{\ell!(k-2\ell)!} 2^{k-2\ell-1} g^{(k-2\ell)} \\ &= \sum_{\ell=0}^{\lfloor \frac{k}{2} \rfloor} (-1)^\ell \frac{k(k-\ell-1)!}{\ell!} 2^{k-2\ell-1} \left(\frac{1}{2\pi i} \int_{\Gamma} \frac{g(\lambda)}{\lambda^{k-2\ell}} d\lambda \right), \end{aligned} \quad (2.16)$$

where in the last step we have used the Cauchy integral formula. For the expansions with the Bessel functions of the first kind we get exactly the same formula, with $(-1)^\ell$ replaced by 1 in the summand, which is also given in [24, Sec. 9.1].

3. Infinite Arnoldi exponential integrator for (1.1). Consider for the moment a linear (finite-dimensional) homogeneous ODE

$$y'(t) = By(t), \quad y(0) = b \quad (3.1)$$

where $y(t) \in \mathbb{C}^n$, with the solution given by the matrix exponential $y(t) = \exp(tB)b$. Algorithms for (3.1) based on Krylov methods are typically constructed as follows, see [11] and references therein for further details. By carrying out N steps of the Arnoldi process for B and b we obtain the Hessenberg matrix F_N and the orthonormal matrix $Q_{N+1} \in \mathbb{C}^{n \times (N+1)}$ that satisfy the so called Arnoldi relation

$$BQ_N = Q_N F_N + f_{N+1,N} q_{N+1} e_N^T, \quad (3.2)$$

where q_i denotes the i th column of $Q_{N+1} = [q_1, \dots, q_{N+1}] = [Q_N, q_{N+1}]$ and $f_{i,j}$ the i,j element of F_N , and $q_1 = b/\beta$ with $\beta := \|b\|$. The columns of Q_N form an orthogonal basis of the Krylov subspace

$$\mathcal{K}_N(B, b) = \text{span}(b, Bb, \dots, B^{N-1}b).$$

As a consequence of (3.2), the Hessenberg matrix F_N is the projection of B onto the Krylov subspace $\mathcal{K}_N(B, b)$, i.e., $F_N = Q_N^* B Q_N$.

The Krylov approximation of (3.1) is subsequently given by

$$y(t) = \exp(tB)b \approx Q_N \exp(tF_N) e_1 \beta. \quad (3.3)$$

Krylov approximations of the matrix exponential has for instance been used in [6, 18, 23].

The first justification of the proposed algorithm is based on applying a Krylov approximation analogous to (3.3) for the infinite-dimensional homogeneous ODE given in Lemma 1. Although this construction is infinite-dimensional, it turns out that due to the structure of A_∞ and the starting vector $b = [u_0^T, e_1^T]^T \in \mathbb{C}^\infty$, the basis matrix Q_N has a particular structure which can be exploited.

Lemma 5 (Basis matrix structure) Let $Q_N \in \mathbb{C}^{\infty \times N}$ be the matrix generated by the Arnoldi method applied to the infinite matrix A_∞ given by (1.6) and the starting vector $b = [u_0^\top, e_1^\top]^\top \in \mathbb{C}^\infty$. Let $q_{1,j} \in \mathbb{C}^{n+1}$, for $j = 1 \dots N$, be the first $n+1$ rows of Q_N and let $q_{i,j} \in \mathbb{C}$, $i = 2, \dots, j = 2, \dots, N$ correspond to the rows $n+2, n+3, \dots$. Then, the basis matrix Q_N has the block-triangular structure

$$Q_N = \begin{bmatrix} q_{1,1} & q_{1,2} & \cdots & q_{1,N} \\ 0 & q_{2,2} & \cdots & q_{2,N} \\ \vdots & 0 & \ddots & \vdots \\ \vdots & 0 & q_{N,N} & \\ & \vdots & 0 & \\ & & \vdots & \end{bmatrix} \in \mathbb{C}^{\infty \times N} \quad (3.4)$$

Proof. The proof can be done by induction. For $N = 1$ the statement is trivial. If we assume Q_N has the structure (3.4), at step N the Arnoldi method will generate a new vector $q_{:,N+1} \in \mathbb{C}^\infty$ which is a linear combination of $A_\infty q_{:,N}$ and the columns of Q_N . Due to the fact that H_∞ is a Hessenberg matrix, and A_∞ has the structure (1.6), $A_\infty q_{:,N}$ will have one more non-zero element than $q_{:,N}$. This completes the proof. \square

The zero-structure in the basis matrix Q_N revealed in Lemma 5, suggests that we can implement the Arnoldi method for (2.2) by only storing the non-zero part of Q_N . By noting that the orthogonalization also preserves the basis matrix structure, we can derive an algorithm where in every step the basis matrix is expanded by a column and a row. We note that the infinite Arnoldi method for nonlinear eigenvalue problems has a similar property [15, Section 5.1]. The proposed algorithm is specified in Algorithm 1. As is common for the Arnoldi method, in Step 7 we used reorthogonalization if necessary.

Another natural procedure to compute a solution to (1.1) would be to truncate the matrix H_∞ and thereby A_∞ such that we obtain a linear finite-dimensional ODE

$$\tilde{v}'(t) = A_m \tilde{v}(t), \quad \tilde{v}(0) = \begin{bmatrix} u_0 \\ e_1 \end{bmatrix}$$

using (1.5) and subsequently applying the standard Krylov approximation (3.3) on this finite-dimensional ODE. It turns out that this approach will provide an algorithm equivalent to Algorithm 1, if the truncation parameter is chosen larger or equal to the number of Arnoldi steps. Hence, in addition to the fact that Algorithm 1 can be interpreted as an infinite-dimensional Krylov approximation of (2.2), the algorithm is also equivalent to the finite-dimensional Krylov approximation corresponding to the truncated matrix, if the truncation parameter is chosen larger than the number of steps.

Lemma 6 Consider N steps of the Arnoldi method applied to $A_m \in \mathbb{C}^{(n+m) \times (n+m)}$ with starting vector $b = [u_0^\top, e_1^\top]^\top \in \mathbb{C}^{n+m}$. Let $u_{N,m}$ be the corresponding Krylov approximation, i.e., $u_{N,m} := [I_n \ 0] Q_N \exp(tF_N) e_1 \beta$. Then, for any $m \geq N$, we have $u_N^{IA} = u_{N,m}$.

Proof. This follows directly from the zero-structure of the basis matrix in (3.4), which holds also for finite m , when $m \geq N$. \square

Algorithm 1: The infinite Arnoldi exponential integrator for (1.1)

Input : $u_0 \in \mathbb{C}^n$, $t \in \mathbb{R}$, $w_0, w_1 \dots \in \mathbb{C}^n$

output: The approximation $u_N^{IA} \approx u(t)$

- 1 Let $\beta = \|u_0\|$, $Q_1 = u_0/\beta$, \underline{F}_0 =empty matrix
 - 2 **for** $k = 1, 2, \dots, N$ **do**
 - 3 Let $q_k = Q(:, k) \in \mathbb{C}^{n+k-1}$
 - 4 Compute $w := A_k q_k$
 - 5 Let \underline{Q}_k be Q_k with one zero row added
 - 6 Compute $h = \underline{Q}_k^* w$
 - 7 Compute $w_\perp := w - \underline{Q}_k h$
 - 8 Repeat Step 5-6 if necessary
 - 9 Compute $\alpha = \|w_\perp\|$
 - 10 Let $\underline{F}_k = \begin{bmatrix} \underline{F}_{k-1} & h \\ 0 & \alpha \end{bmatrix}$
 - 11 Let $Q_{k+1} := [\underline{Q}_k, w_\perp/\alpha]$
 - 12 **end**
 - 13 Let $F_N \in \mathbb{R}^{N \times N}$ be the leading submatrix of $\underline{F}_N \in \mathbb{R}^{(N+1) \times N}$
 - 14 Compute the approximation $u_N^{IA} = [I_n \ 0] Q_N \exp(tF_N) e_1 \beta$
-

4. Convergence analysis. We saw in Lemma 6 that although the Algorithm 1 is derived from Arnoldi's method applied to an infinite-dimensional operator A_∞ , the result of N steps of the algorithm can also be interpreted as Arnoldi's method applied to the truncated matrix A_m for any $m \leq N$. In order to study the convergence we will set $m = N$ and use the exact solution associated with the truncated matrix A_N , denoted by $u_N(t)$. More precisely,

$$u_N(t) := [I_n \ 0] \exp(tA_N) u_N. \quad (4.1)$$

By trivial subtraction and triangle inequality we have that the error is bounded by

$$\|u_N^{IA} - u(t)\| \leq \|u(t) - u_N(t)\| + \|u_N(t) - u_N^{IA}\|. \quad (4.2)$$

The first term $\|u(t) - u_N(t)\|$ can be interpreted as an error associated with A_N (the truncation of A_∞) and is not related to Arnoldi's method, whereas the second term $\|u_N(t) - u_N^{IA}\| = \|u_N(t) - u_{N,N}\|$ can be seen as an error associated with the Arnoldi approximation of the matrix exponential. The following two subsections are devoted to the characterization of these two errors.

4.1. Bound for the truncation error. It will turn out that the truncation error (first term in (4.2)) can be analyzed by relating it to $\exp(tH_N)e_1$, i.e., a vector of functions generated by the truncated Hessenberg matrix H_N . Let $\bar{\varepsilon}_N$ denote the difference between the basis functions and the functions generated by the Hessenberg matrix,

$$\bar{\varepsilon}_N(t) := \bar{\phi}_N(t) - \exp(tH_N)e_1, \quad \bar{\phi}_N(t) := \begin{pmatrix} \phi_0(t) \\ \vdots \\ \phi_{N-1}(t) \end{pmatrix}. \quad (4.3)$$

The following lemma shows that a sufficient condition for the convergence of the first term in (4.2) is that $\|W_N \bar{\varepsilon}_N(s)\| \rightarrow 0$. The following subsections are devoted to the analysis of $\|W_N \bar{\varepsilon}_N(s)\|$ for different basis functions, and in particular lead up the convergence of the truncation error given under general conditions in Theorem 8 and Theorem 11.

Lemma 7 *Let u be the solution to the ODE (1.1) and u_N be defined as in (4.1). Suppose the expansion (1.2) is uniformly convergent with respect to s . Then,*

$$\begin{aligned} \|u(t) - u_N(t)\| &\leq \int_0^t \|e^{(t-s)A}\| \|g(s) - W_N e^{sH_N} e_1\| ds \leq \\ &\int_0^t \|e^{(t-s)A}\| ds \left(\max_{s \in [0,t]} \|g(s) - W_N \bar{\phi}_N(s)\| + \max_{s \in [0,t]} \|W_N \bar{\varepsilon}_N(s)\| \right). \end{aligned} \quad (4.4)$$

Moreover, for every $s \leq t$ we have

$$\|g(s) - W_N \bar{\phi}_N(s)\| \rightarrow 0 \quad \text{as } N \rightarrow \infty. \quad (4.5)$$

Proof. The first bound in (4.4) follows from the variation-of-constants formula $u(t) = e^{tA}u_0 + \int_0^t e^{(t-s)A}g(s) ds$, which gives the exact solution for the ODE (1.1), and from the representation [10, pp. 248]

$$\begin{aligned} u_N &= [I_n \quad 0] e^{tA_N} u_N = [I_n \quad 0] \begin{bmatrix} e^{tA} & \int_0^t e^{(t-s)A} W_N e^{sH_N} ds \\ 0 & e^{tH_N} \end{bmatrix} u_N \\ &= e^{tA} u_0 + \int_0^t e^{(t-s)A} W_N e^{sH_N} e_1 ds. \end{aligned}$$

The second inequality follows by adding and subtracting $\bar{\phi}_N(s)$. The limit expression (4.5) follows from the fact that $g(s) - W_N \bar{\phi}_N(s) = \sum_{\ell=N}^{\infty} W_\ell \phi_\ell(s)$, which is the remainder term in the expansion (1.2). The limit vanishes due to the fact that (1.2) is uniformly convergent. \square

4.1.1. Bounds on $\|W_N \bar{\varepsilon}_N\|$: scaled monomial basis. Suppose ϕ_ℓ are scaled monomials such that H_N is a transposed Jordan matrix, i.e., the truncation of (1.4). The definition of $\bar{\varepsilon}_N$ yields $\bar{\varepsilon}_N^{(k)}(0) = \bar{\phi}_N^{(k)}(0) - H_N^k e_1$. It follows from the structure (1.4) that, for $k \leq N$, $H_N^k e_1 = e_k$ and $H_N^k e_1 = 0$ if $k > N$. Moreover, $\bar{\phi}_N^{(k)}(0) = e_k \phi_k^{(k)}(0) = e_k$ if $k \leq N$ and $\bar{\phi}_N^{(k)}(0) = 0$ if $k > N$. Hence, $\bar{\varepsilon}_N^{(k)}(0) = 0$ for all k . Since $\bar{\varepsilon}_N$ is analytic and all derivatives vanish, $\bar{\varepsilon}_N(t) \equiv 0$. Hence, we have obtained the following result.

Theorem 8 *Suppose $\bar{\phi}_N$ are the scaled monomials, given by $\phi_\ell(t) := t^\ell / \ell!$, and $H_N \in \mathbb{R}^{N \times N}$ is the leading submatrix of (1.4). Then,*

$$\bar{\varepsilon}_N(t) \equiv 0$$

where $\bar{\varepsilon}_N(t)$ is given by (4.3). Consequently, if the basis functions are the scaled monomials, the truncation error $\|u(t) - u_N(t)\| \rightarrow 0$ independent of t .

4.1.2. Bounds on $\|W_N \bar{\varepsilon}_N\|$: Bessel basis functions. If the basis functions are Bessel functions or modified Bessel functions of the first kind, further analysis is required to show that $\|W_N \bar{\varepsilon}_N\|$ vanishes. The elements of $\bar{\varepsilon}_N$, denoted by $\varepsilon_{N,k}$, $k = 0, \dots, N-1$, can be bounded as follows.

Lemma 9 *Let $H_N \in \mathbb{R}^{N \times N}$ be defined as either (2.4) or (2.6). Then, the vector $\bar{\varepsilon}_N$ satisfies*

$$\bar{\varepsilon}_N(t) = \int_0^t e^{(t-s)H_N} J_N(s) e_N ds \quad (4.6)$$

and is bounded as follows.

(a) For all $t \geq 0$,

$$\|\bar{\varepsilon}_N(t)\| \leq \frac{\left(\frac{1}{2}t\right)^N}{(N+1)!} \sqrt{2}te^t. \quad (4.7)$$

(b) Suppose $t \geq 2$. Then there exists a constant $\tilde{C}(t)$ depending only on t such that for $1 \leq k \leq N$,

$$|\varepsilon_{N,k}(t)| \leq \tilde{C}(t) \frac{t^k}{2^{2N-k}} \frac{(N-k)!}{(2N-k+1)!}. \quad (4.8)$$

Proof. Proof of (4.6): From the properties (2.3) we see that $\bar{J}_N(t)$ satisfies the initial value problem $\bar{J}'_N(t) = H_N \bar{J}_N(t) + J_N(t)e_N$, $J(0) = e_1$. Therefore, the error $\bar{\varepsilon}_N(t) := \bar{J}_N(t) - e^{tH_N} e_1$ satisfies the initial value problem $\bar{\varepsilon}'_N(t) = H_N \bar{\varepsilon}_N + J_N(t)e_N$, $\bar{\varepsilon}_N(0) = 0$, for which the solution is given by (4.6).

The statement (4.7) follows from properties of H_N and Bessel functions as follows. From Lemma 17, we have that $\|e^{(t-s)H_N}\| \leq \sqrt{2}e^{t-s}$ and therefore

$$\|\bar{\varepsilon}_N(t)\| \leq \int_0^t \|e^{(t-s)H_N}\| |J_N(s)| ds \leq \sqrt{2} \int_0^t e^{(t-s)} \frac{\left(\frac{1}{2}s\right)^N}{N!} e^s ds = \frac{\left(\frac{1}{2}t\right)^N}{(N+1)!} \sqrt{2}te^t,$$

where in the last step we used that for $t > 0$, $|\phi_N(t)| \leq \frac{\left|\frac{1}{2}t\right|^N}{N!} e^t$ if $\phi_N = J_N$ or $\phi_N = I_N$, which is a consequence of the formula [24, pp. 49],

$$|J_n(z)| \leq \frac{\left|\frac{1}{2}z\right|^n}{n!} e^{|Im(z)|}. \quad (4.9)$$

It remains to show (4.8). We first note that, (4.9) and Lemma 18 with $R = t^2$ implies that

$$|\varepsilon_{N,k}(t)| = \left| \int_0^t e_k^T e^{(t-s)H_N} e_N J_N(s) ds \right| \leq \frac{e^t C(t^2)}{t^{2(N-k)} N! 2^{2N-k}} \int_0^t s^N (t-s)^{N-k} ds, \quad (4.10)$$

where $C(t^2)$ is given by (A.4). We identify the integral on right-hand side of (4.10) as a scaled Beta function $t^{m+n+1} B(m+1, n+1)$. The conclusion (4.8) now follows from the application of a formula for $B(m+1, n+1)$ in [1, pp. 258]. More precisely,

$$|\varepsilon_{N,k}(t)| \leq \frac{e^t C(t^2)}{t^{2(N-k)} N! 2^{2N-k}} \frac{t^{2N-k+1} N! (N-k)!}{(2N-k+1)!} = e^t C(t^2) \frac{t^{k+1}}{2^{2N-k}} \frac{(N-k)!}{(2N-k+1)!}.$$

□

We have now derived a bound on $\bar{\varepsilon}_N$ and shown that $\|\bar{\varepsilon}_N(t)\| \rightarrow 0$ as $N \rightarrow \infty$, when the basis functions are the Bessel functions or the modified Bessel functions of the first kind. Note that this does not necessarily imply that $\|W_N \bar{\varepsilon}_N(t)\| \rightarrow 0$, since the coefficient matrix W_N may not be bounded for all N . Fortunately, the analyticity of $g(t)$ gives us a bound on the growth of the coefficients w_k .

Lemma 10 Suppose g is analytic in a neighborhood of a disc of radius t centered at the origin. Let M_t be defined as

$$M_t = \max_{|\lambda|=t} \|g(\lambda)\|. \quad (4.11)$$

Let the vectors w_k be the coefficients of the expansion (1.2) of $g(t)$, where the functions ϕ_ℓ are the Bessel or the modified Bessel functions of the first kind. Then, for $0 \leq t < 2$ we have the bound

$$\|w_k\| \leq M_t k! \left(\frac{2}{t}\right)^k \quad \text{for all } k \geq 0. \quad (4.12)$$

Moreover, for $t \geq 2$, we have the bounds

$$\|w_k\| \leq M_t k! 2 \left(\frac{2}{t}\right)^k \quad \text{for all } k \geq 0, \quad (4.13)$$

and

$$\|w_k\| \leq M_t k! 2 \left(\frac{2}{t}\right)^k \quad \text{for all } k > \left(\frac{t}{2}\right)^2 + 1. \quad (4.14)$$

Proof. The closed form (2.16) for the coefficients w_k implies that for all $k \geq 0$

$$\|w_k\| \leq \sum_{\ell=0}^{\lfloor \frac{k}{2} \rfloor} \frac{k(k-\ell-1)!}{\ell!} 2^{k-2\ell-1} \left\| \frac{1}{2\pi i} \int_{\Gamma} \frac{g(\lambda)}{\lambda^{k-2\ell+1}} d\lambda \right\|. \quad (4.15)$$

Combining (4.11) and (4.15) gives us

$$\|w_k\| \leq \frac{M_t}{2} \sum_{\ell=0}^{\lfloor \frac{k}{2} \rfloor} \frac{k(k-\ell-1)!}{\ell!} \left(\frac{2}{t}\right)^{k-2\ell}. \quad (4.16)$$

Thus, when $t < 2$, we have that for all $k \geq 0$

$$\|w_k\| \leq \frac{M_t}{2} \left(\frac{2}{t}\right)^k \sum_{\ell=0}^{\lfloor \frac{k}{2} \rfloor} \frac{k(k-\ell-1)!}{\ell!} \leq \frac{M_t}{2} \left(\frac{2}{t}\right)^k 2k!$$

which gives (4.12). When $t \geq 2$, $\left(\frac{2}{t}\right)^{k-2\ell} \leq 1$ if $0 \leq \ell \leq \lfloor \frac{k}{2} \rfloor$, and with a similar reasoning (4.13) follows from (4.16).

In order to show (4.14), we note that (4.16) can be expressed as

$$\|w_k\| \leq \frac{M_t}{2} \sum_{\ell=0}^{\lfloor \frac{k}{2} \rfloor} c_\ell, \quad (4.17)$$

where $c_0 = k! \left(\frac{2}{t}\right)^k$ and $c_\ell = \frac{1}{(k-\ell)\ell} \left(\frac{t}{2}\right)^2 \cdot c_{\ell-1}$ if $\ell \geq 1$. When $1 \leq \ell \leq \lfloor \frac{k}{2} \rfloor$, $(k-\ell)\ell \geq k-1$, and we see that c_ℓ satisfies $c_\ell \leq a_k c_{\ell-1}$ such that $c_\ell \leq a_k^\ell c_0$, where $a_k = t^2/4(k-1)$. The conclusion (4.14) follows from (4.17) and the fact that the assumption $k > 2 \left(\frac{t}{2}\right)^2 + 1$ implies that $a_k < 1/2$ and by taking the limit $\ell \rightarrow \infty$. \square

By combining the bound of $\bar{\varepsilon}_N$ and the bound of w_ℓ we arrive at the following result for $W_N \bar{\varepsilon}_N(t)$.

Theorem 11 *If W_N corresponds to the expansion of $g(t)$ with the Bessel functions or the modified Bessel functions of the first kind, then for all $t > 0$*

$$\|W_N \bar{\varepsilon}_N(t)\| \rightarrow 0, \quad \text{as } N \rightarrow \infty. \quad (4.18)$$

Consequently, if the basis functions are the Bessel functions or the modified Bessel functions, the truncation error $\|u(t) - u_N(t)\| \rightarrow 0$ independent of t .

Proof. Consider first the case $0 \leq t < 2$. By (4.7) and (4.12) we see that

$$\begin{aligned} \left\| \sum_{\ell=0}^N w_\ell \varepsilon_{N,\ell}(t) \right\| &\leq \|\bar{\varepsilon}_N(t)\| \sum_{k=0}^N \|w_k\| \leq \|\bar{\varepsilon}_N(t)\| \sum_{k=0}^N M_t k! \left(\frac{2}{t}\right)^k \\ &\leq \frac{\left(\frac{t}{2}\right)^N}{(N+1)!} \sqrt{2} t e^t M_t \left(\frac{2}{t}\right)^N (N! + (N-1)! + \dots + 1) \\ &= \sqrt{2} t M_t \left(\frac{1}{N+1} + \frac{1}{(N+1)N} + \dots + \frac{1}{(N+1)!} \right) \leq \sqrt{2} t M_t \left(2 \frac{1}{N+1} \right). \end{aligned}$$

Consider the case $t \geq 2$. Suppose $N > \tilde{k} := \left\lceil 2 \left(\frac{t}{2}\right)^2 + 1 \right\rceil$. We see that

$$\left\| \sum_{\ell=0}^N w_\ell \varepsilon_{N,\ell}(t) \right\| \leq \sum_{\ell=0}^{\tilde{k}} \|w_\ell\| |\varepsilon_{N,\ell}(t)| + \sum_{\ell=\tilde{k}+1}^N \|w_\ell\| |\varepsilon_{N,\ell}(t)|. \quad (4.19)$$

We now show that both of the terms in the right-hand side of (4.19) vanish as $N \rightarrow \infty$. Using the bound (4.13) of Lemma 10, and the bound (4.8) of Lemma 9 with $k = \ell$, we see that there exists a constant $\tilde{C}_2(t) := M_t \tilde{C}(t) t^{\tilde{k}}$, which are independent of N , such that

$$\sum_{\ell=0}^{\tilde{k}} \|w_\ell\| |\varepsilon_{N,\ell}(t)| \leq \tilde{C}_2(t) \sum_{\ell=0}^{\tilde{k}} \frac{\ell!(N-\ell)!}{2^{2N-\ell}(2N-\ell+1)!}. \quad (4.20)$$

Since for $\ell \leq \tilde{k} \leq N$, $\ell!(N-\ell)! < (\ell+1)!(N-\ell)! \leq (N+1)!$ and $2^{2N-\ell}(2N-\ell+1)! \geq 2^N((N-\tilde{k})+N+1)!$, we see that

$$\frac{(\ell+1)!(N-\ell)!}{2^{2N-\ell}(2N-\ell+1)!} \leq \frac{(N+1)!}{2^N((N-\tilde{k})+N+1)!} \leq \frac{1}{2^N N^{N-\tilde{k}}}. \quad (4.21)$$

By inserting (4.21) into (4.20) we conclude that the first term in (4.19) vanishes as $N \rightarrow \infty$.

For the second term of (4.19), we use the bound (4.14) of Lemma 10, and the bound (4.8), to see that there exists a constant $\tilde{C}_3(t) := M_t \tilde{C}(t)$, which are independent of N , such that

$$\begin{aligned} \sum_{\ell=\tilde{k}+1}^N ||w_\ell|| |\varepsilon_{N,\ell}(t)| &\leq C_3(t) \sum_{\ell=\tilde{k}+1}^N \left(\frac{2}{t}\right)^\ell \frac{t^\ell}{2^{2N-\ell}} \frac{\ell!(N-\ell)!}{(2N-\ell+1)!} \\ &\leq C_3(t) \sum_{\ell=\tilde{k}+1}^N \frac{N!}{(2N-\ell+1)!} \\ &\leq C_3(t) \left((N-\tilde{k}-1) \cdot \frac{1}{(N+2)(N+1)} + \frac{1}{N+1} \right), \end{aligned}$$

This implies that the second term in the right-hand side of (4.19) converges to zero as $N \rightarrow \infty$ and completes the proof. \square

4.2. Error bounds for the Arnoldi approximation. In order to show convergence of (4.2) we will now study the second term in (4.2). Let

$$Q_N = \begin{bmatrix} Q_{1,N+1} \\ Q_{2,N+1} \end{bmatrix} \in \mathbb{C}^{(n+N+1) \times (N+1)},$$

where $Q_{1,N} \in \mathbb{C}^{n \times N}$ is the orthonormal matrix and $F_N = Q_N^* A_N Q_N$ the Hessenberg matrix given by the infinite Arnoldi algorithm after N iterations. The Arnoldi relation (3.2), with $B = A_N$, implies that

$$\begin{aligned} A Q_{1,N} + W Q_{2,N} &= Q_{1,N} F_N + f_{N+1,N} q_{1,N+1} e_N^T \\ H_N Q_{2,N} &= Q_{2,N} F_N + f_{N+1,N} q_{2,N+1} e_N^T. \end{aligned} \tag{4.22}$$

The polynomial approximation property of the Arnoldi method [19, Lemma 3.1] states that for any polynomial p of degree less than N we have $p(A_N)u_N = \beta Q_N p(F_m)e_1$. In our situation we can exploit the structure of A_N when we select $p(z) = z^\ell$. From the second block of $p(A_N)u_N$ we conclude that $H_N^\ell e_1 \beta^{-1} = Q_{2,N} F_N^\ell e_1$ for all $\ell \leq N-1$. By stacking this equation as columns into a matrix equation we find that $K_N(H_N, e_1)\beta^{-1} = Q_{2,N} K_N(F_N, e_1)$, such that

$$Q_{2,N} = K_N(H_N, e_1) K_N(F_N, e_1)^{-1} \beta^{-1}, \tag{4.23}$$

where K_N denotes the Krylov matrix, defined in (2.7). The orthonormality of Q_N implies that $\|Q_N\| = 1$, from which it follows that $\|Q_{1,N}\| \leq 1$ and $\|Q_{2,N}\| \leq 1$. Consider A_N of the form (1.6) for a general Hessenberg matrix H_N . The infinite Arnoldi approximation at step N is given by

$$[I_n \quad 0] Q_N \exp(tF_N) e_1 \beta = Q_{1,N} \exp(tF_N) e_1 \beta, \tag{4.24}$$

where $\beta = \|u_N\|$. We again use the polynomial approximation property, which implies that $\sum_{\ell=0}^{N-1} \frac{1}{\ell!} A_N^\ell = Q_N \sum_{\ell=0}^{N-1} \frac{1}{\ell!} F_N^\ell \beta$. Hence, the second term in the error (4.2) can be expressed as

$$u_N(t) - u_N^{IA}(t) = [I_n \quad 0] (\exp(tA_N)u_N - Q_N \exp(tF_N) e_1 \beta) = a_N + b_N, \tag{4.25}$$

where

$$a_N := [I_n \ 0] r_N(tA_N) u_N \quad (4.26)$$

$$b_N := -Q_{1,N} r_N(tF_N) e_1 \beta \quad (4.27)$$

and r_N denotes the remainder term in the truncated Taylor expansion. We will use an explicit representation of r_N ,

$$r_N(z) = \sum_{\ell=N}^{\infty} \frac{z^\ell}{\ell!} = z^N \varphi_N(z), \quad (4.28)$$

with the standard definition of φ -functions,

$$\varphi_\ell(z) := \sum_{k=0}^{\infty} \frac{z^k}{(k+\ell)!} = \int_0^1 e^{(1-\tau)z} \frac{\tau^{\ell-1}}{(\ell-1)!}. \quad (4.29)$$

4.2.1. Convergence of a_N in (4.25). The analysis of (4.25) is separated into analysis of a_N and b_N . We first need a reformulation of a_N .

Lemma 12 *Let A_N , u_N , r_N and φ_ℓ be defined as above. Then, the following expression holds*

$$\begin{aligned} a_N &= (tA)^N \varphi_N(tA) u_0 + \sum_{\ell=1}^N t^\ell (tA)^{N-\ell} \varphi_N(tA) g^{(\ell-1)}(0) \\ &\quad + \sum_{\ell=N+1}^{\infty} t^\ell \varphi_\ell(tA) W_N H_N^{\ell-1} e_1. \end{aligned} \quad (4.30)$$

Proof. By induction it is readily verified from (1.6) that

$$A_N^k \begin{bmatrix} u_0 \\ e_1 \end{bmatrix} = \begin{bmatrix} A^k u_0 + \sum_{\ell=1}^k A^{k-\ell} W_N H_N^{\ell-1} e_1 \\ H_N^k e_1 \end{bmatrix}.$$

From this it follows that

$$\begin{aligned} [I_n \ 0] r_N(tA_N) \begin{bmatrix} u_0 \\ e_1 \end{bmatrix} &= [I_n \ 0] \sum_{k=N}^{\infty} \frac{(tA_N)^k}{k!} \begin{bmatrix} u_0 \\ e_1 \end{bmatrix} \\ &= \sum_{k=N}^{\infty} \frac{(tA)^k}{k!} u_0 + \sum_{k=N}^{\infty} \sum_{\ell=1}^k t^\ell \frac{(tA)^{k-\ell}}{k!} W_N H_N^{\ell-1} e_1 \\ &= \sum_{k=N}^{\infty} \frac{(tA)^k}{k!} u_0 + \sum_{\ell=1}^N \sum_{k=N}^{\infty} t^\ell \frac{(tA)^{k-\ell}}{k!} W_N H_N^{\ell-1} e_1 + \sum_{\ell=N+1}^{\infty} \sum_{k=\ell}^{\infty} t^\ell \frac{(tA)^{k-\ell}}{k!} W_N H_N^{\ell-1} e_1. \end{aligned} \quad (4.31)$$

Since $W_N H_N^{\ell-1} e_1 = g^{(\ell-1)}(0)$ when $0 \leq \ell \leq N$, we find for the second term on the last line of (4.31) that

$$\sum_{\ell=1}^N \sum_{k=N}^{\infty} t^\ell \frac{(tA)^{k-\ell}}{k!} W_N H_N^{\ell-1} e_1 = \sum_{\ell=1}^N t^\ell (tA)^{N-\ell} \varphi_N(tA) g^{(\ell-1)}(0).$$

For the third term on the last line of (4.31) we see that

$$\sum_{\ell=N+1}^{\infty} \sum_{k=\ell}^{\infty} t^{\ell} \frac{(tA)^{k-\ell}}{k!} W_N H_N^{\ell-1} e_1 = \sum_{\ell=N+1}^{\infty} t^{\ell} \varphi_{\ell}(tA) W_N H_N^{\ell-1} e_1,$$

from which the claim follows. \square

We are now ready to state convergence of the first term in (4.25) under general assumptions about the nonlinearity g .

Theorem 13 *Let A_N be defined as in (1.6). Assume that for the vectors $g^{(\ell)}(0)$ are bounded by*

$$\|g^{(\ell)}(0)\| \leq c \|A\|^{\ell} \quad (4.32)$$

for some constant $c \in \mathbb{R}$. Then, a_N defined by (4.26) satisfies

$$a_N \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

Proof. We bound the norm of the term (4.30) as

$$\begin{aligned} \| [I_n \quad 0] r_N(tA_N) u_N \|_2 &\leq \|(tA)^N \varphi_N(tA) u_0\| + \left\| \sum_{\ell=1}^N t^{\ell} (tA)^{N-\ell} \varphi_N(tA) g^{(\ell-1)}(0) \right\| \\ &+ \left\| \sum_{\ell=N+1}^{\infty} t^{\ell} \varphi_{\ell}(tA) W_N H_N^{\ell-1} e_1 \right\|. \end{aligned} \quad (4.33)$$

By Lemma 19 we get a bound for the first term in (4.33) as

$$\|(tA)^N \varphi_N(tA) u_0\| \leq \frac{\|tA\|^N \max(1, e^{\mu(tA)})}{N!} \|u_0\|.$$

For the second term in (4.33), we see that

$$\begin{aligned} \left\| \sum_{\ell=1}^N t^{\ell} (tA)^{N-\ell} \varphi_N(tA) g^{(\ell-1)}(0) \right\| &\leq \sum_{\ell=1}^N t^{\ell} \|tA\|^{N-\ell} \|g^{(\ell-1)}(0)\| \|\varphi_N(tA)\| \\ &\leq \tilde{C} \sum_{\ell=1}^N \|tA\|^N \frac{\max(1, e^{\mu(tA)})}{N!} = \tilde{C} \|tA\|^N \frac{\max(1, e^{\mu(tA)})}{(N-1)!}, \end{aligned}$$

where $\tilde{C} = C/\|tA\|$. Thus, also the second term in (4.33) converges to zero as $N \rightarrow \infty$.

For the third term in (4.33), we use Lemmas 19 and 20 to find that

$$\begin{aligned} \left\| \sum_{\ell=N+1}^{\infty} t^{\ell} \varphi_{\ell}(tA) W_N H_N^{\ell-1} e_1 \right\| &\leq \sum_{\ell=N+1}^{\infty} t^{\ell} \|\varphi_{\ell}(tA)\| \|G_N\| \|K_N(H_N, e_1)^{-1} H_N^{\ell-1} e_1\| \\ &\leq \sum_{\ell=N+1}^{\infty} t^{\ell} \frac{\max(1, e^{\mu(tA)})}{\ell!} \|G_N\| 2\sqrt{N} (1 + \sqrt{2})^N \\ &= t^{N+1} \varphi_{N+1}(t) \max(1, e^{\mu(tA)}) 2\sqrt{N} (1 + \sqrt{2})^N \|G_N\| \\ &\leq \frac{t^{N+1} e^t \max(1, e^{\mu(tA)}) 2\sqrt{N} (1 + \sqrt{2})^N \|G_N\| e^t}{(N+1)!}. \end{aligned}$$

By assumption (4.32),

$$\|G_N\| \leq \|G_N\|_F = \sqrt{\sum_{\ell=0}^{N-1} \|g^{(\ell-1)}(0)\|^2} \leq C \sqrt{\sum_{\ell=0}^{N-1} \|A\|^{2\ell}} = C \sqrt{\frac{\|tA\|^{2N} - 1}{\|tA\|^2 - 1}}.$$

Thus also the third term in (4.33) converges to zero as $N \rightarrow \infty$. \square

4.2.2. Convergence of b_N in (4.25). Bounding the remainder $Q_{1,N}r_N(tF_N)e_1\beta$ in the error expression (4.25) needs in general additional assumptions about F_N . Before stating the convergence theorem, we need the following lemma.

Lemma 14 Assume that $1 < \|H_N\| < \|A\|$ and that (4.32) is satisfied for some constant $c > 0$. Then, for $0 \leq \ell \leq N$

$$\|F_N^\ell e_1\| \leq (1 + \beta^{-1}c\ell)\|A\|^\ell.$$

Proof. From (1.6), (2.9) and (4.23) we see that the Hessenberg matrix F_N is given by

$$\begin{aligned} F_N &= Q_N^* A_N Q_N = Q_{1,N}^* A Q_{1,N} + Q_{2,N}^* H_N Q_{2,N} + Q_{1,N}^* W_N Q_{2,N} \\ &= Q_{1,N}^* A Q_{1,N} + Q_{2,N}^* H_N Q_{2,N} + \beta^{-1} Q_{1,N}^* G_N K_N(F_N, e_1)^{-1}, \end{aligned}$$

where $G_N = [g(0) \ g'(0) \ \dots \ g^{(N-1)}(0)]$. Thus, for the norms of the products $F_N^\ell e_1$, $1 \leq \ell \leq N$, we get the following recursion:

$$\begin{aligned} \|F_N^\ell e_1\| &\leq \| (Q_{1,N}^* A Q_{1,N} + Q_{2,N}^* H_N Q_{2,N}) F_N^{\ell-1} e_1 \| \\ &\quad + \beta^{-1} \|Q_{1,N}^* G_N K_N(F_N, e_1)^{-1} F_N^{\ell-1} e_1\| \\ &\leq \max(\|A\|, \|H_N\|) \|F_N^{\ell-1} e_1\| + \beta^{-1} \|Q_{1,N}^* g^{(\ell-1)}(0)\| \\ &\leq \|A\| \|F_N^{\ell-1} e_1\| + \beta^{-1} c \|A\|^{\ell-1}, \end{aligned}$$

since $\beta > 1$ and $K_N(F_N, e_1)^{-1} F_N^{\ell-1} e_1 = e_\ell$ for $1 \leq \ell \leq N$. By induction we have that

$$\|F_N^\ell e_1\| \leq \|A\|^\ell \|F_N^0 e_1\| + \beta^{-1} c \ell \|A\|^{\ell-1} = \|A\|^\ell + \beta^{-1} c \ell \|A\|^{\ell-1} \leq \|A\|^\ell (1 + \beta^{-1} c \ell).$$

\square

We are ready to give the following result, which gives sufficient conditions for the convergence of the Arnoldi error.

Theorem 15 (Arnoldi error) Suppose there exists a constant $c > 0$ such that (4.32) is satisfied. Suppose Algorithm 1 generates a Hessenberg matrix F_N such that for some constant C , $\|F_N^N\| \leq C^N$ for all $N > 0$. Then, b_N given by (4.27) satisfies

$$\|b_N\| \rightarrow 0 \text{ as } N \rightarrow \infty.$$

Moreover, the Arnoldi error in (4.25) satisfies

$$\|u_N(t) - u_N^{IA}(t)\| \rightarrow 0 \text{ as } N \rightarrow \infty.$$

Proof. We see from (4.28) that

$$r_N(tF_N)e_1 = \sum_{\ell=N}^{\infty} \frac{(tF_N)^\ell e_1}{\ell!} = \sum_{k=1}^{\infty} (tF_N)^{Nk} \left(\sum_{\ell=0}^{N-1} \frac{(tF_N)^\ell e_1}{(kN+\ell)!} \right). \quad (4.34)$$

We see by Lemma 14 that

$$\begin{aligned} \left\| \sum_{\ell=0}^{N-1} \frac{(tF_N)^\ell e_1}{(kN+\ell)!} \right\| &\leq \sum_{\ell=0}^{N-1} \frac{(1+c\ell)\|tA\|^\ell}{(kN+\ell)!} \leq (1+\beta^{-1}cN) \sum_{\ell=0}^{N-1} \frac{\|tA\|^\ell}{(kN+\ell)!} \\ &\leq (1+\beta^{-1}cN)\varphi_{kN}(t\|A\|) \leq (1+\beta^{-1}cN) \frac{e^{t\|tA\|}}{(kN)!}. \end{aligned} \quad (4.35)$$

In the last inequality above we use Lemma 19. Thus, we see from (4.34) and (4.35) that

$$\begin{aligned} \|b_N\| &\leq \|Q_N\| \|r_N(tF_N)e_1\| \beta \leq \sum_{k=1}^{\infty} \left(\|(tF_N)^N\|^k \left\| \sum_{\ell=0}^{N-1} \frac{(tF_N)^\ell e_1}{(kN+\ell)!} \right\| \right) \beta \\ &\leq (\beta + cN) \sum_{k=1}^{\infty} \frac{e^{t\|tA\|} \|(tF_N)^N\|^k}{(kN)!} \beta \leq (\beta + cN) e^{t\|tA\|} \sum_{k=1}^{\infty} \frac{(tC)^{kN}}{(kN)!} \beta \end{aligned}$$

which converges to zero as $N \rightarrow \infty$. \square

Remark 16 (Assumptions in Theorem 15) Theorem 15 is only applicable when there exists a constant C such that $\|F_N^N\| \leq C^N$ for all $N > 0$, where F_N is the Hessenberg matrix generated by Algorithm 1. This is a restriction on the generality of our convergence theory. In our numerical experiments we have seen no indication that the assumption should not be satisfied (see Figure 5.2c). Moreover, the assumption can be motivated by certain intuitive uniformity assumptions and the generic behavior of Arnoldi's method for eigenvalue problems, as follows. From the definition of the spectral radius, we have

$$\|F_N^\ell\|^{1/\ell} \rightarrow \rho(F_N) \quad \text{as } \ell \rightarrow \infty. \quad (4.36)$$

Moreover, under the condition that the Arnoldi method approximates the largest eigenvalue of A_∞ , we also have

$$\rho(F_N) \rightarrow \rho(A_\infty) \quad \text{as } N \rightarrow \infty. \quad (4.37)$$

The operator $\rho(A_\infty)$ is block diagonal and the (1,1)-block is a finite operator A and the (2,2)-block is a bounded operator (by assumption (1.3b)). Hence, it is natural to assume that $\rho(A_\infty) = d \in \mathbb{R}$ exists. If $\rho(A_\infty)$ exists and the limits (4.36) and (4.37) hold also in a uniform sense, we have that $\|F_N^N\|^{1/N} \rightarrow d$, which implies the assumption.

5. Numerical examples.

5.1. Numerical evaluation of the derivatives $g^{(\ell)}(0)$. In order to carry out N steps of the algorithm, we need the expansion coefficients w_0, \dots, w_N , which are directly available from the derivatives $g^{(\ell)}(0)$, $\ell = 0, \dots, N$ via (2.9). If the nonlinearity is not explicit such it is not possible to compute expressions for the derivatives by hand, there are several alternatives. One may use, e.g., symbolic differentiation which is available for several special functions in MATLAB or the techniques of *automatic differentiation* can be used [9].

Another alternative is to use matrix functions. If an efficient and numerically stable matrix function implementation of $h(z)$ is available (see, e.g., [10, Ch. 4]), one

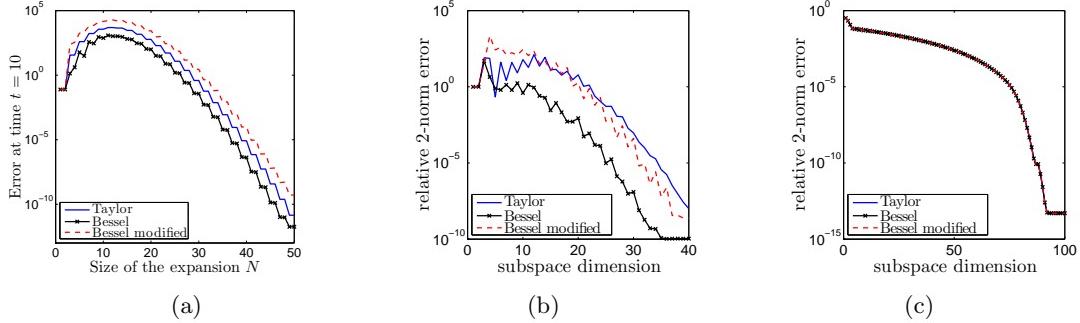


Fig. 5.1: Subfigure (a) shows the absolute error vs. expansion size N for the approximation of $f(t) = \sin^2(t)$ for the three different choices of basis functions. Subfigure (b) and (c) shows the error vs. the Krylov subspace size for the Schrödinger example. (b) $\epsilon = 10^{-5}$, $T = 10$, (c) $\epsilon = 10^{-3}$, $T = 0.5$.

may use the fact that

$$h(H) e_1 = \begin{bmatrix} h(0) \\ h'(0) \\ h''(0)/2 \\ \vdots \\ h^{(N-1)}(0)/N! \end{bmatrix} \quad \text{for } H = \begin{bmatrix} 0 & & & \\ 1 & 0 & & \\ & \ddots & \ddots & \\ & & 1 & 0 \end{bmatrix} \in \mathbb{R}^{N \times N}.$$

Also, there exists methods to compute derivatives by numerically integrating the contour integral in the Cauchy integral formula [4].

5.2. 1-D Schrödinger equation with inhomogeneity. We first consider a finite difference spatial discretization (with 100 points) of the initial value problem

$$i\partial_t u = -\epsilon\partial_{xx} u + f(t) \sin(2^4\pi x(1-x)), \quad x \in [0, 1], \quad t \in [0, T] \quad (5.1)$$

subject to periodic boundary conditions, with $f(t) = (1+i)\sin(t)^2$ and initial condition $u(x, 0) = \exp(-100(x-0.5)^2)$. Figure 5.1a depicts the absolute error of the approximation $f(t) \approx W_N \exp(tH_N) e_1 = \sum_{\ell=0}^{N-1} w_\ell \phi_\ell^{(N)}(t)$, for the three different choices of W_N and H_N , for $1 \leq N \leq 50$ and $t = 6$. We again compare the infinite Arnoldi algorithm approximation of $u(T)$ for the three different expansions of $f(t)$. In Figures 5.1 we illustrate the relative 2-norm error of the approximations vs. the Krylov subspace size, when $\epsilon = 10^{-5}$ and $\epsilon = 10^{-3}$. In Fig. 5.1a we observe different truncation errors for different basis functions. Analogously, a difference in convergence speed of Alg. 1 can be observed in Fig. 5.1b.

In a sense, the convergence of the linear part (associated with A) dominates the total error in the case of the strong linear part ($\epsilon = 10^{-3}$), and therefore the choice of basis does not affect the convergence, which is also observed in Fig. 5.1c.

We illustrate the competitiveness of the approach in terms of CPU-time¹ in Figures 5.2, when $\epsilon = 10^{-5}$ and $\epsilon = 10^{-3}$. We use three different integrators: the infinite

¹All experiments are carried out on a desktop computer with a 2.90 GHz single Pentium processor using MATLAB.

Arnoldi algorithm with the Bessel functions of the first kind and the MATLAB implementations of the Runge-Kutta method `ode45` and `ode15s`.

Note that the Matlab integrators use adaptive time-stepping, and that the infinite Arnoldi method performs a single time step for which the subspace size is set a priori. When $\epsilon = 10^{-5}$, `ode45` needed 10,16,25,40,86 time steps to obtain the results of Figure 5.2, and `ode15s` 10,13,51,96,189, respectively. When $\epsilon = 10^{-3}$, `ode45` needed 29,30,31,33,33 time steps, and `ode15s` 10,15,22,60,124 time steps.

When the linear part is not very stiff, we see that the explicit integrator `ode45` gives better results than the stiff implicit solver `ode23`. For this particular simulation setup, the infinite Arnoldi method is faster than the MATLAB Runge-Kutta implementations, as can be observed in Figures 5.2.

Figure 5.2c gives a numerical justification for the assumptions used in the error analysis given in Section 4.2.2. We consider the numerical example above with the parameter $\epsilon = 10^{-3}$. We observe that up to machine precision, $\|F_N^N\|^{1/N} \rightarrow \rho(A)$ as $N \rightarrow \infty$, such that the conditions discussed in Remark 16 appear to be satisfied.

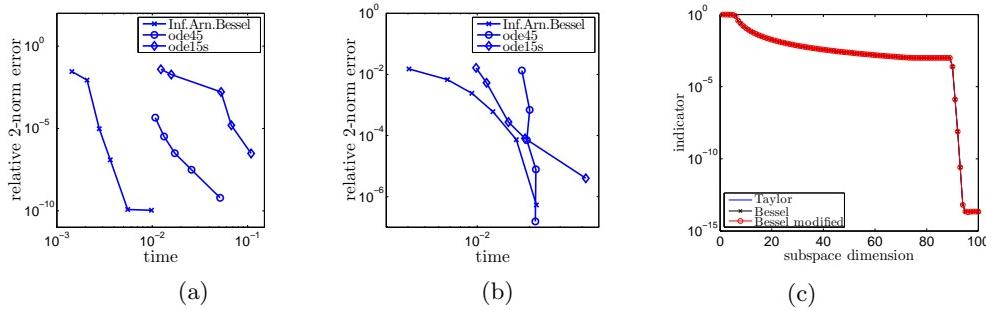


Fig. 5.2: Subfigures (a) and (b) show the error vs. CPU time in seconds for the 1-D Schrödinger example, with (a) $\epsilon = 10^{-5}$, $T = 10$, and (b) $\epsilon = 10^{-3}$, $T = 0.5$. Subfigure (c) show the indicator $\|F_N^N\|^{1/N}/\rho(A) - 1$

5.3. 2-D Schrödinger equation with inhomogeneity. In order to illustrate generality of the infinite Arnoldi method, we consider a finite difference spatial discretization (with 100^2 points) of the two-dimensional initial value problem

$$i\partial_t u = -\epsilon(\partial_{xx}u + \partial_{yy}u) + f(t) \sin(2^4\pi x(1-x)y(1-y)), \quad x \in [0, 1], \quad t \in [0, T] \quad (5.2)$$

subject to periodic boundary conditions, with $f(t)$ as in (5.1) and initial condition $u(x, 0) = \exp(-100((x - 0.5)^2 + (y - 0.5)^2))$

We compare the infinite Arnoldi algorithm approximation of $u(T)$ for the three different expansion of $f(t)$. Figures 5.3 depict the relative 2-norm error of the approximations vs. the Krylov subspace size, when $\epsilon = 5 \cdot 10^{-3}$ and $\epsilon = 5 \cdot 10^{-2}$. We see again that the convergence of the linear part starts to dominate the total error as the linear part gets larger.

Figures 5.4 depict the relative 2-norm errors of the approximations of $u(t)$ vs. the CPU time when $\epsilon = 5 \cdot 10^{-2}$ and $\epsilon = 5 \cdot 10^{-3}$, for the three different integrators: infinite Arnoldi with Bessel expansion and Matlab codes `ode45` and `ode15s`.

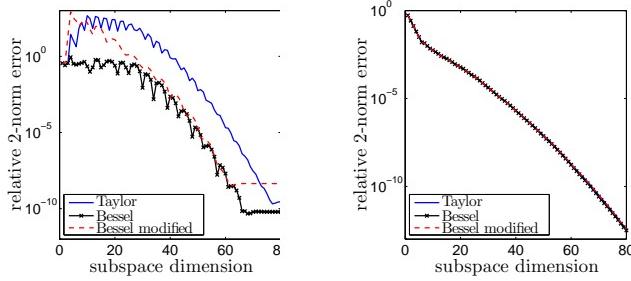


Fig. 5.3: Error vs. the Krylov subspace size for the Schrödinger example. Left: $\epsilon = 5 \cdot 10^{-3}$, $T = 10$, right: $\epsilon = 5 \cdot 10^{-2}$, $T = 0.25$.

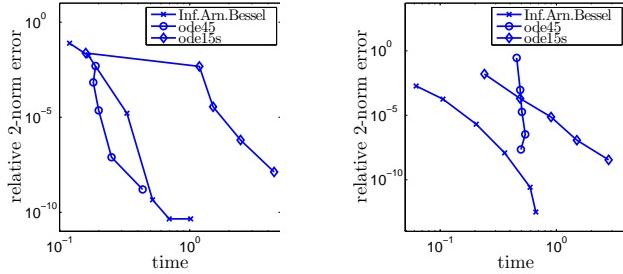


Fig. 5.4: Error vs. CPU time in seconds for the 2-D Schrödinger example. Left: $\epsilon = 5 \cdot 10^{-3}$, $T = 10$, right: $\epsilon = 5 \cdot 10^{-2}$, $T = 0.25$.

6. Concluding remarks and outlook. The main contribution of this paper is a new algorithm for inhomogeneous linear ODEs and the associated convergence theory. The algorithm belongs to a class of methods *exponential integrators*. Many of the techniques that are combined with exponential integrators are likely feasible in this situation. For instance, a potentially faster approach can be derived by repeating the algorithm for different t , i.e., instead of integrating to $t = T$ directly, the algorithm can be applied for h_1, \dots, h_m where $T = h_1 + \dots + h_m$. Moreover, it seems also feasible to apply the algorithm to certain nonlinear equations, by simple linearization procedure, although it would certainly not be efficient for all nonlinear problems. See [14] for variants of exponential integrators.

Acknowledgments. The authors thank Stefan Güttel for several valuable discussions.

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Appendix A. Additional results needed in proofs.

Lemma 17 *Let $H_N \in \mathbb{R}^{N \times N}$ be defined as in (2.4) or as in (2.6), and let the eigen-decomposition of H_N be given as $H_N = V\Lambda V^{-1}$. Then, the condition number of the eigenvector matrix in 2-norm, i.e., $\kappa_2(V) = \|V\| \|V^{-1}\|$, is given by $\kappa_2(V) = \sqrt{2}$. Moreover,*

$$\|e^{tH_N}\| \leq \sqrt{2} e^{t\alpha(H_N)}, \quad (\text{A.1})$$

where $\alpha(A)$ denotes the spectral abscissa of A . If H_N is given by (2.4), $\alpha(H_N) = 0$ and if H_N is given by (2.6) we have that $\alpha(H_N) \leq 1$.

Proof. We first consider the case where H_N is defined by (2.6). Note that H_N is the colleague matrix of the Chebyshev polynomial $T_N(x)$ [22, Theorem 18.1], and we know that H_N has N different eigenpairs (λ, v) where λ -values are the zeros of $T_N(x)$, and v -vectors are of the form $v = [T_0(\lambda) \dots T_{N-1}(\lambda)]^T$. Thus, H_N has the eigendecomposition $H_N = V\Lambda V^{-1}$, where

$$V = \begin{bmatrix} T_0(t_0) & \dots & T_0(t_{N-1}) \\ \vdots & & \vdots \\ T_{N-1}(t_0) & \dots & T_{N-1}(t_{N-1}) \end{bmatrix},$$

and (t_0, \dots, t_{N-1}) are the N different zeros of $T_N(\cdot)$. The Chebyshev polynomials satisfy a discrete orthogonality condition

$$\sum_{k=0}^{N-1} T_i(t_k) T_j(t_k) = \begin{cases} 0 & , \quad i \neq j \\ N & , \quad i = j = 0 \\ N/2 & , \quad i = j \neq 0. \end{cases} \quad (\text{A.2})$$

With (A.2) we verify that VV^* is a diagonal matrix where all elements are equal to $N/2$ except the first element which is equal to N . Hence, R -matrix in the QR-decomposition of $V^* = QR$ is a diagonal matrix and we conclude that there exists $Q \in \mathbb{R}^{n \times n}$ such that $QQ^* = Q^*Q = I$ and $V = \alpha \operatorname{diag}(\sqrt{2}, 1, \dots, 1)Q^*$, where $\alpha = \sqrt{N/2}$. We see that $\|V\| = |\alpha|\sqrt{2}$, and $\|V^{-1}\| = 1/|\alpha|$. Therefore $\kappa_2(V) = \sqrt{2}$.

Let now H_N be defined as in (2.4). Define the polynomials $\tilde{T}_n(x)$, $n \geq 0$ as $\tilde{T}_n(x) = i^n T_n(-ix)$, where T_n is the n th Chebyshev polynomial. We now use the recurrence relation of Chebyshev polynomials; see, e.g., [22, Chapter 3]. We see that \tilde{T}_i satisfies $\tilde{T}_0(x) = 1$, $\tilde{T}_1(x) = x$ and $\tilde{T}_{n+1}(x) = -2x\tilde{T}_n(x) + \tilde{T}_{n-1}(x)$. Therefore, the eigenvalues of H_N are the zeros of the polynomial $\tilde{T}_n(x)$, which are i multiplied with the zeros of the polynomial $T_n(x)$. The corresponding eigenvectors are of the form $v = [\tilde{T}_0(\lambda) \dots \tilde{T}_{n-1}(\lambda)]^T$. From the condition (A.2) it follows that the polynomials $\tilde{T}_i(x)$ satisfy the condition

$$\sum_{k=0}^{N-1} T_i(t_k) T_j(t_k) = \begin{cases} 0 & , \quad i \neq j \\ N & , \quad i = j = 0 \\ i^{i+j} N/2 & , \quad i = j \neq 0 \end{cases}$$

and the rest of the proof follows as for the modified Bessel functions. The bound (A.1) follows from the fact that $\|e^{tH_N}\| = \|Ve^{t\Lambda}V^{-1}\| \leq \kappa(V)\|e^{t\Lambda}\|$. The conclusion about the spectral abscissa if H_N is given by (2.6) follows from Gershgorin's theorem and the conclusion of if H_N is given by (2.4) follows from the fact that the eigenvalues of H_N are imaginary. \square

Lemma 18 *Let H_N be defined either as (2.4) or (2.6) and let $t > 0$. Let $R \in \mathbb{R}$ be any value such that $R > t$. Then, the elements of e^{tH_N} are bounded as*

$$(e^{tH_N})_{i,j} \leq C(R) \lambda^{|i-j|}, \quad (\text{A.3})$$

where $\lambda = \frac{t}{2R}$ and

$$C(R) = \max(\|\exp(tH_N)\|, 2\sqrt{2} \frac{e^{R+\frac{1}{4R}}}{1-\lambda}). \quad (\text{A.4})$$

Proof. We may apply directly the bound (3.10) in [3, Sec. 3.7]. We know that tH_N has its spectrum inside the interval $[-t, t]$, which has the logarithmic capacity $\rho = t/2$. For the integration contour we take the same ellipse as in [3], so $V = 2\pi$ and $M(R) = e^{R+\frac{1}{4R}}$, where $R > t$ can be chosen freely. Let $H_N = VDV^{-1}$ be the diagonalization of H_N . From Lemma 17 we know that $\kappa(V) = \sqrt{2}$. The bound (3.10) of [3] gives (A.3). \square

Lemma 19 For any matrix $A \in \mathbb{C}^{n \times n}$ and positive integer ℓ ,

$$\|\varphi_\ell(A)\| \leq \frac{\max(1, e^{\mu(A)})}{\ell!},$$

where $\mu(A)$ denotes the logarithmic norm, i.e., $\mu(A) = \max\{\lambda : \lambda \in \Lambda(\frac{A+A^*}{2})\}$.

Proof. From (4.29) we see that

$$\|\varphi_\ell(A)\| = \left\| \int_0^1 e^{(1-t)A} \frac{t^{\ell-1}}{(\ell-1)!} dt \right\| \leq \int_0^1 \|e^{(1-t)A}\| \frac{t^{\ell-1}}{(\ell-1)!} dt.$$

Using the Dahlquist bound $\|e^A\| \leq e^{\mu(A)}$ and the fact that $\mu((1-t)A) \leq \max\{0, \mu(A)\}$ for $0 \leq t \leq 1$, the claim follows. \square

Lemma 20 Let H_N be defined as in (2.4) or (2.6). Then, for $k \geq N$,

$$\|K_N(H_N, e_1)^{-1} H_N^k e_1\| \leq 2\sqrt{N}(1 + \sqrt{2})^N. \quad (\text{A.5})$$

Proof. Let $p_N(\lambda) = \sum_{\ell=0}^N \alpha_\ell \lambda^\ell$ be the characteristic polynomial of H_N . Define

$$\tilde{\alpha}_N = - \begin{bmatrix} \alpha_0 \\ \vdots \\ \alpha_{N-1} \end{bmatrix}, \quad \text{and} \quad C(\tilde{\alpha}_N) = \begin{bmatrix} 1 & & & \tilde{\alpha}_N \\ & \ddots & & \\ & & 1 & \end{bmatrix} \in \mathbb{R}^{N \times N}.$$

Suppose $k \geq N$. Since $H_N^N e_1 = -\sum_{\ell=0}^{N-1} \alpha_\ell H_N^\ell e_1 = K_N(H_N, e_1) \tilde{\alpha}_N$, we see that

$$H_N K_N(H_N, e_1) = [H_N e_1 \quad \dots \quad H_N^N e_1] = K_N(H_N, e_1) C(\tilde{\alpha}_N),$$

and since $H_N^{N-1} e_1 = K_N(H_N, e_1) e_N$, we see that

$$H_N^k e_1 = H_N^{k-N+1} K_N(H_N, e_1) e_N = K_N(H_N, e_1) C(\tilde{\alpha}_N)^{k-N+1} e_N,$$

i.e.,

$$K_N(H_N, e_1)^{-1} H_N^k e_1 = C(\tilde{\alpha}_N)^{k-N+1} e_N. \quad (\text{A.6})$$

We recognize that $C(\tilde{\alpha}_N)$ is the companion matrix of the N th Chebyshev polynomial T_N , and that $V_N C(\tilde{\alpha}_N) = \Lambda_N V_N$, where $\lambda_1, \dots, \lambda_N$ are the zeroes of T_N , $\Lambda_N = \text{diag}(\lambda_1, \dots, \lambda_N)$ and V_N is the Vandermonde matrix corresponding to $\lambda_1, \dots, \lambda_N$, i.e.,

$$V_N = \begin{bmatrix} 1 & \lambda_1 & \dots & \lambda_1^{N-1} \\ \vdots & \vdots & & \vdots \\ 1 & \lambda_N & \dots & \lambda_N^{N-1} \end{bmatrix}.$$

Thus for $\ell \geq 1$, $C(\tilde{\alpha}_N)^\ell = V_N^{-1} \Lambda_N^\ell V_N$, and subsequently for any matrix norm $\|\cdot\|_*$

$$\|C(\tilde{\alpha}_N)^\ell\|_* \leq \|V_N^{-1}\|_* \|\Lambda_N^\ell\|_* \|V_N\|_* \leq \|V_N^{-1}\|_* \|V_N\|_* \quad \text{for all } \ell \geq 1, \quad (\text{A.7})$$

since $|\lambda_i| \leq 1$ for all $1 \leq i \leq N$. From [7, Thm. 4.3 and Example 6.2], we know that

$$\|V_N^{-1}\|_\infty \|V_N\|_\infty \leq 2(1 + \sqrt{2})^N. \quad (\text{A.8})$$

Thus, using (A.6), we see that for $k \geq N$ $\|K_N(H_N, e_1)^{-1} H_N^k e_1\| \leq \|C(\tilde{\alpha}_N)^{k-N+1}\| \leq \sqrt{N} \|C(\tilde{\alpha}_N)^{k-N+1}\|_\infty$ and the statement follows from (A.7) and (A.8). \square